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An Assessment of Some Existing and Proposed Klein-Nishina Monte Carlo Sampling Methods

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ABSTRACT

An exact Monte Carlo non-uniform rejection technique is developed for sampling the Klein-Nishina distributions for scattered photon secondary energy. This method samples with nearly 100% efficiency at high incident photon energies where other rejection methods tend to extremely low efficiency. The efficiency and computing speed is compared with those of other sampling methods. The accuracy of one approximate method is evaluated by comparing the exact and approximate probability distribution functions.

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I. INTRODUCTION

Monte Carlo simulation of photon scattering in a continuous energy domain requires selection of the secondary energy and the scattering angle cosine (μ) at each scattering collision. The probability density function (p.d.f.) which describes this distribution is the Klein-Nishina distribution,

$$\tilde{p}(x,\mu) = [\mu^2 - 1 + x + \frac{1}{x}]/G \qquad \xi \leq x \leq 1, \quad -1 \leq \mu \leq 1 \tag{1}$$

where x is the ratio of α' (the secondary energy in units of electron rest mass energy) to α (the incident photon energy), G is a normalization constant, and the minimum possible secondary energy is $\xi = 1/(1 + 2\alpha)$. For a given α, each scattering angle corresponds uniquely to a secondary energy:

$$\mu = 1 + \frac{1}{\alpha} - \frac{1}{\alpha x} \, . \tag{2}$$

In general, the difficulty in sampling the Klein-Nishina p.d.f. stems from its algebraic complexity and from the radically dissimilar shapes at high and low energies, as shown in Figures 1 and 2. We shall examine here several techniques from two distinct classes of Klein-Nishina sampling methods.

II. ANALYTICAL APPROXIMATION

To sample the Klein-Nishina p.d.f. directly, one first eliminates the scattering angle cosine using Eq. (2) to reduce $\tilde{p}(x,\mu)$ to

$$p(x) = \left[x + \alpha^{-2} \, \xi^{-1} + \frac{1}{\alpha^2} \, (\alpha^2 - 2\alpha - 2) \, \frac{1}{x} + \frac{1}{\alpha^2 \, x^2} \right] / G. \tag{3}$$

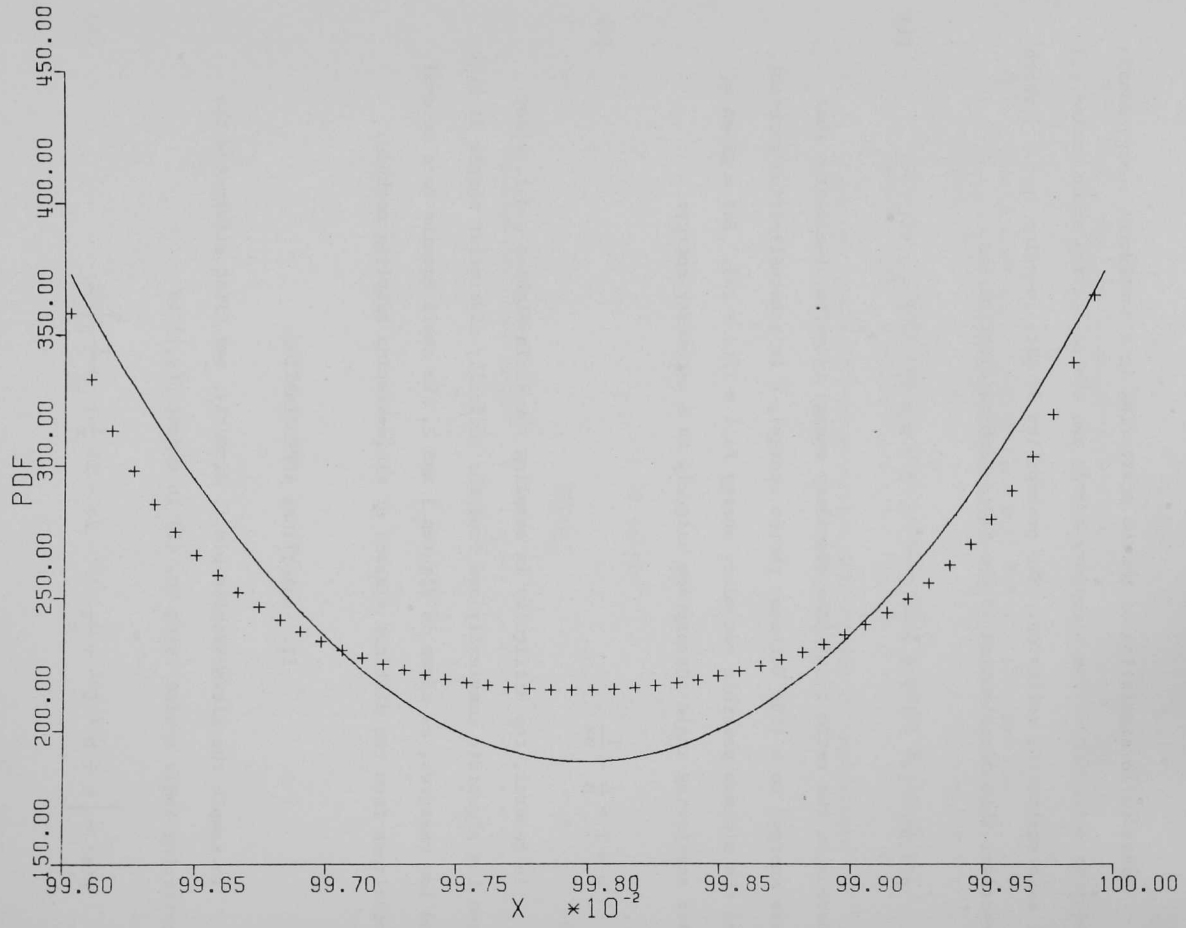

Fig. 1 The Klein-Nishina Distribution p(x) for $\alpha = 0.002$, and the Sample Distribution (+), q(x), from the Approximate Inverse Method.[3]

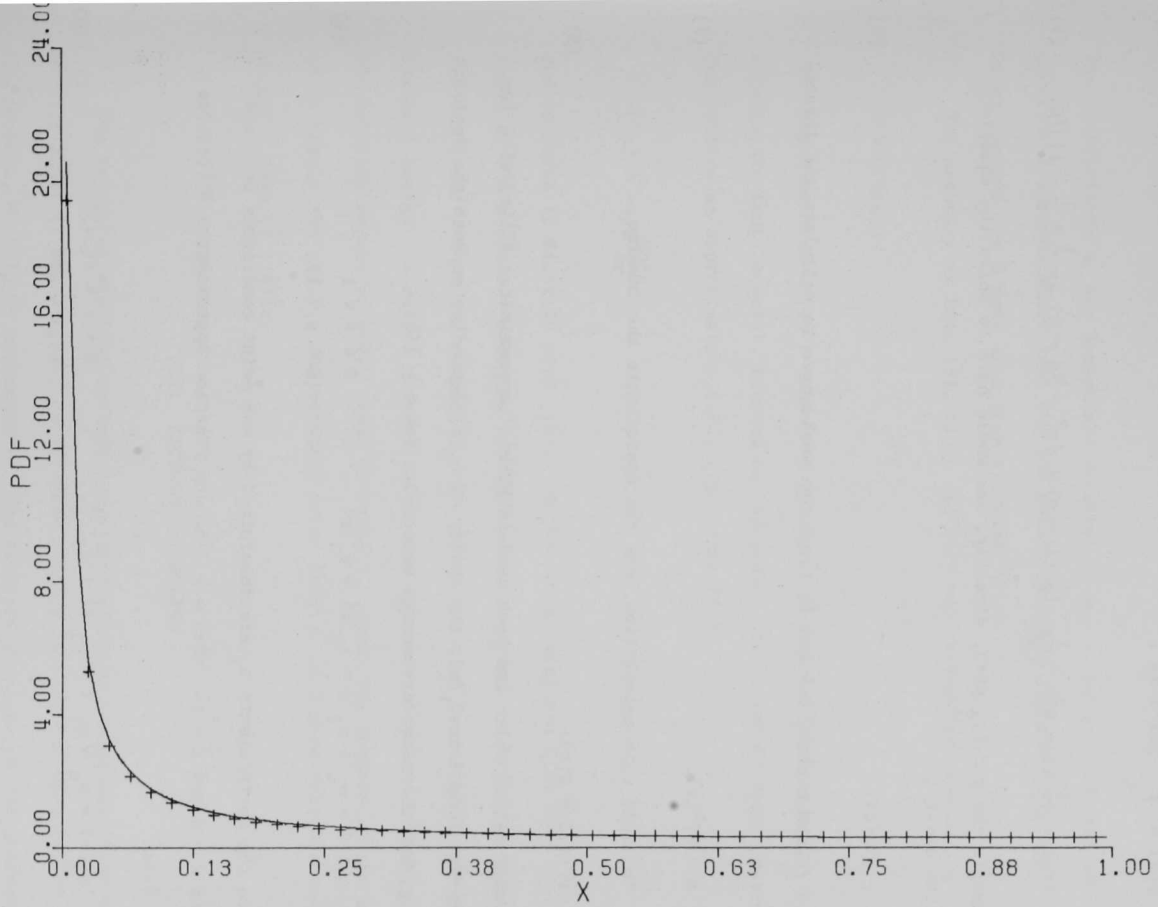

Fig. 2 The Klein-Nishina Distribution p(x) for α = 200., and the Sample Distribution (+), q(x), from the Approximate Inverse Method.[3]

The c.d.f. is formed by

$$P(x) = \int_x^1 p(x')\,dx', \tag{4}$$

or

$$P(x) = \{\frac{1}{2}(1 - x^2) + \frac{1}{\alpha^2}\,[\frac{1}{\xi}(1 - x) + (\alpha^2 - 2\alpha - 2)\ln\frac{1}{x} + \frac{1}{x} - 1]\}/G. \tag{5}$$

To sample the p.d.f., p(x), directly, one would have to solve the equation for the c.d.f.,

$$r = P(x), \tag{6}$$

for a random number, $0 \leq r \leq 1$, i.e., one would have to calculate the inverse function,

$$x = P^{-1}(r). \tag{7}$$

To avoid this calculation, one can approximate the inverse,

$$P^{-1}(r) \approx Q(r). \tag{8}$$

One such method which has been used in MCNP[2,3] approximates $P^{-1}(r)$ with two different functions $Q_i(r)$, the choice of $Q_i(r)$ depending on both the incident energy and the secondary energy selected. For $\alpha \leq 7/6$,

$$Q_1(r) = a_o + a_1 r + a_2 r^2 + a_3 r^3, \qquad \begin{matrix} 0 \leq r \leq 1 \\ (\xi \leq x \leq 1) \end{matrix} \tag{9}$$

where the coefficients a_i are determined by end point conditions on Q and Q' at $x = \xi$ and $x = 1$. When $\alpha > 7/6$, one function approximates $P^{-1}(r)$ for $x \geq 0.3$,

$$Q_1(r) = a_o + a_1 r + a_2 r^2 + a_3 r^3, \qquad \begin{matrix} 0 \leq r \leq P(0.3) \\ (0.3 \leq x \leq 1) \end{matrix} \tag{10}$$

and a second function is used for $x < 0.3$,

$$Q_2(r) = 0.3\ e^{-\Lambda[r - P(0.3)]} \qquad P(0.3) \leq r \leq 1 \quad (\xi \leq x \leq 0.3) \tag{11}$$

The coefficients a_i are determined as above at $x = 1$ and $x = 0.3$, and the constant Λ is determined from the end point condition imposed on Q_2 at $x = \xi$. Other recipes for Q have also been proposed.[4, 5, 6, 7]

The accuracy of Eqs. (9), (10), and (11) was tested[3] by calculating

$$\tilde{x} = Q(P(x))$$

and comparing $\tilde{x}$ to x for a number of x-values at each incident energy. An alternative test, however, focuses on the p.d.f., p(x), rather than the c.d.f. One derives an approximate p.d.f., q(x), from Q(r),

$$q(x) = -1/[\frac{dQ(r)}{dr}],\ x \equiv Q(r), \tag{12}$$

and compares it directly with p(x). In this work, p(x) and q(x) were calculated at 100 secondary energies for each of a wide range of incident energies. Figures 1 and 2 show the comparisons between p and q at two extreme values of incident energy. A better perspective on the accuracy is gained by evaluating the relative errors of q(x), shown in Table 1. Since the purpose of the method is to sample the p.d.f., the relative error in q(x) is a more reliable indicator of error than $(\tilde{x} - x)/x$.

III. REJECTION SAMPLING

The rejection sampling methods comprise a class of techniques which can be very powerful for sampling complicated p.d.fs, because the calculation of the inverse, Eq (7), is unnecessary. The simplest of these is the uniform

Table I. Maximum Magnitude Errors

α	$\frac{q(x) - p(x)}{p(x)}$	$\frac{(\tilde{x} - x)}{x}$
.002	.143	7.6×10^{-5}
.02	.143	8.2×10^{-4}
.2	.151	.011
2.	.138	.023
20.	.096	.013
200.	.123	.028

rejection method.[8] The sampling efficiency, E, or fraction of samples accepted, is given by

$$E = \frac{1}{M(1 - \xi)} \tag{13}$$

where M is the maximum value of p(x) on $(\xi,1)$. Figure 3 shows E approaching 2/3 as α becomes small, but for large α, M increases and the efficiency tends to zero.

The efficiency of rejection sampling can be improved by drawing candidate samples from a non-uniform distribution, g(x). If g(x) is simple, its c.d.f. can be inverted analytically, and if it approximates p(x) well, the efficiency will be high. Horowitz, et. al,[9] proposed a linear g(x) which improved the efficiency by a factor of two over the uniform method, but only at high energies where the efficiency is prohibitively small (Figure 3).

A more elaborate non-uniform method was developed earlier by Kahn,[8] who proposed a simultaneous sampling method utilizing two independent component p.d.f's of a non-linear g(x). The Klein-Nishina p.d.f. is rewritten using the transformation $z = 1/x$,

$$h(z) = \frac{1}{Kz^2}\left(\mu^2 + \frac{1}{z} + z - 1\right), \qquad 1 \leq z \leq \frac{1}{\xi}, \tag{14}$$

where

$$\mu = 1 + \frac{1}{\alpha} - \frac{z}{\alpha}\,. \tag{15}$$

Since both

$$g_1(z) = \frac{K_1}{Kz^2}\left(\mu^2 + \frac{1}{z}\right) \tag{16}$$

and

$$g_2(z) = \frac{K_2}{Kz^2}(z - 1) \tag{17}$$

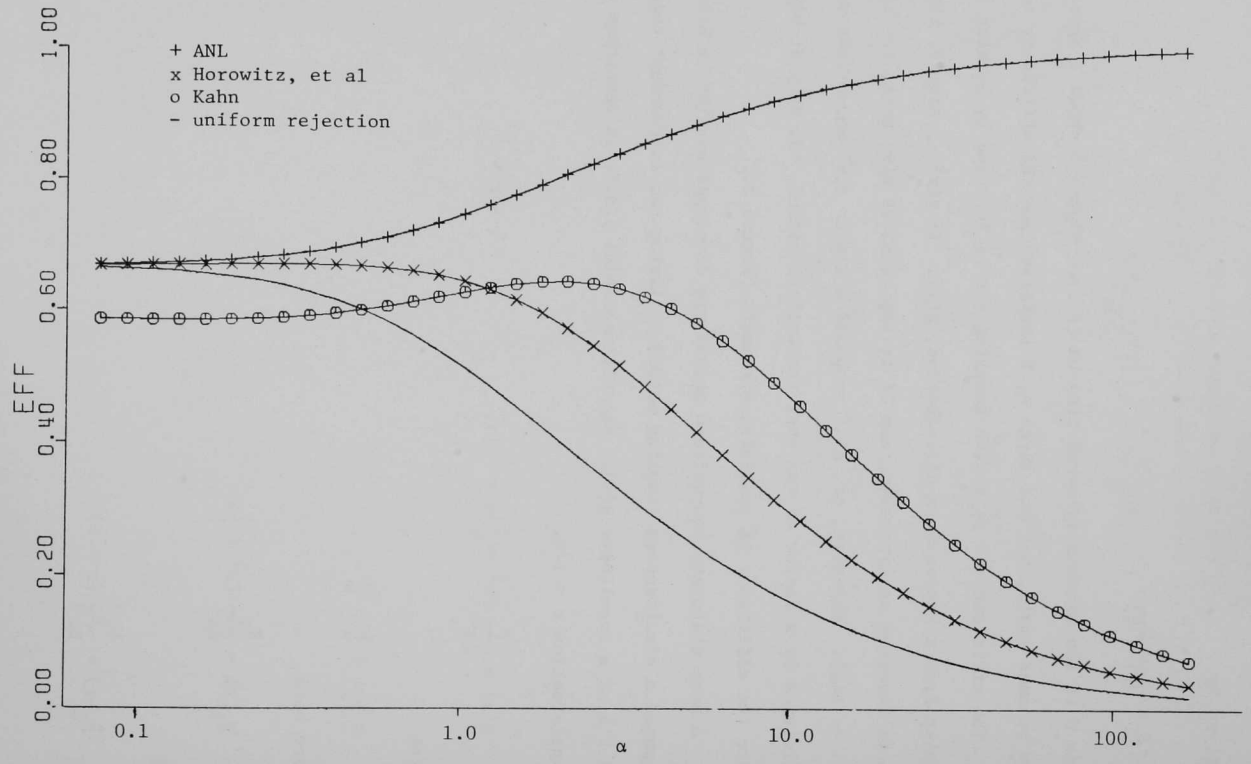

Fig. 3 Rejection Method Sampling Efficiencies Over a Range of Incident Energies (α).

are non-negative on $1 \leq z \leq \frac{1}{\xi}$, they can each be sampled as p.d.fs. After eliminating μ, one draws candidate samples, z, for rejection from either g_1 or g_2 with the appropriate probability and then accepts with the probability $h(z) = Kz^2/[g_1(z)/K_1 + g_2(z)/K_2]$. As shown in Figure 3, however, E again tends to zero for high incident energy photons.

By recasting Eq. 3 in the form,

$$p(x) = [x + \frac{1}{x} + \frac{1}{\alpha^2}\,(1 - \frac{1}{x})\,(\frac{1}{\xi} - \frac{1}{x})]/G, \tag{18}$$

a second approximating p.d.f. is suggested,

$$g(x) = (x + \frac{1}{x})/G'. \tag{19}$$

Since $\xi \approx 1$ for small α, g(x) is approximately uniform on $\xi \leq x \leq 1$. For large α, p(x) - g(x) is very small, and the efficiency tends to 1.0. Equivalent to sampling from g(x) is sampling from one of the two component p.d.fs of g(x),

$$g_1(x) = \frac{1}{1 - \xi^2}\,x \tag{20}$$

with probability

$$\pi_1 = \frac{1}{2}\,(1 - \xi^2)/[\frac{1}{2}\,(1 - \xi^2) + \ln\frac{1}{\xi}], \tag{21}$$

and from the second component p.d.f.,

$$g_2(x) = \frac{1}{x \ln\frac{1}{\xi}}\,, \tag{22}$$

for the remainder. Figure 3 constrasts the efficiency at high energy of Eq. (19) with those of the other methods discussed above.

In this work, timing comparisons were made on the IBM 3033 among the methods discussed above. The computing speeds, shown in Figure 4, are a result both of the efficiencies and of the number and type of arithmetic operations required by for each candidate. Although the efficiency of Kahn's method is lowest over part of the energy range, each candidate sample requires substantially less time to formulate because no special functions (SQRT,ALOG, etc.) must be evaluated. At high energy, however, the efficiency of each method becomes the dominant influence on computing speed, so the method proposed above in Eq. (19) is faster than Kahn's. Horowitz's method requires evaluation of special functions in order to achieve modestly increased sampling efficiency, and is therefore slower than uniform rejection. It is also apparent from Figure 4 that there is no computing speed advantage gained by using the approximate inverse method.

IV. CONCLUSIONS

The approximate inverse method used in MCNP samples from a distribution with substantial approximation errors, but without any corresponding advantage in computing speed. Improvement of rejection sampling efficiency must require excessive arithmetic. Kahn's non-linear rejection method is the fastest of the methods studied up to 10 MeV because the relatively low efficiency is more than compensated for by the small number of arithmetic operations required per candidate sample. Above 10 MeV, however, Kahn's low sampling efficiency overwhelms the arithmetic advantage. Since the proposed rejection method is highly efficient at high energy, the optimum technique seems to be Kahn's nonlinear method below 10 MeV, and the proposed rejection method here at higher energies.

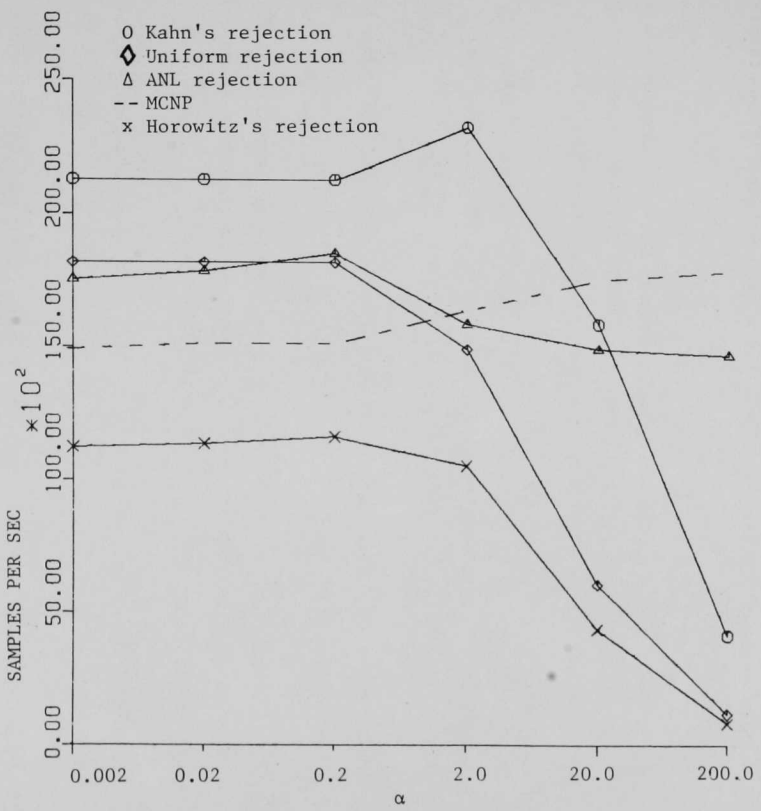

Fig. 4 Computing Speeds of Four Rejection Methods and an Approximate Inverse Method Over a Range of Incident Energies (α).

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